



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:30 PM GMT

PDB ID : 1PYG  
Title : STRUCTURAL BASIS FOR THE ACTIVATION OF GLYCOGEN PHOSPHORYLASE B BY ADENOSINE MONOPHOSPHATE  
Authors : Sprang, S.  
Deposited on : 1992-07-07  
Resolution : 2.87 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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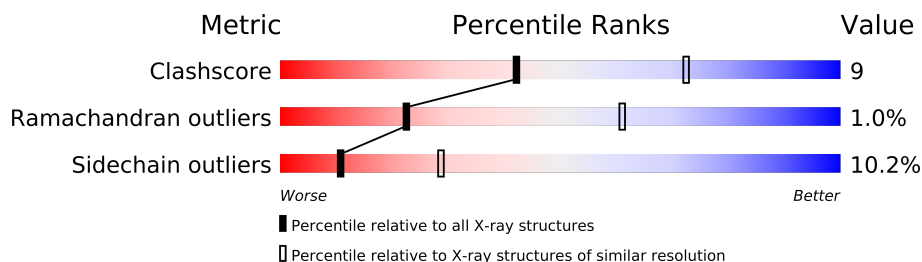
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1696 (2.90-2.86)
Ramachandran outliers	78287	1647 (2.90-2.86)
Sidechain outliers	78261	1650 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
1	B	842	
1	C	842	
1	D	842	

## 2 Entry composition i

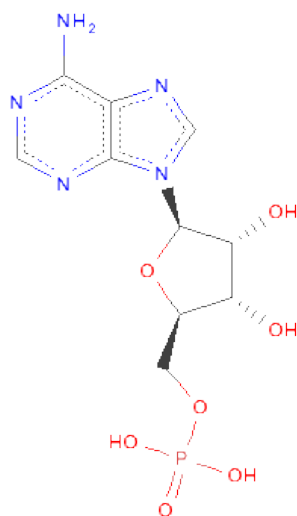
There are 3 unique types of molecules in this entry. The entry contains 26214 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			
1	B	791	Total	C	N	O	S	0	0	0
			6434	4099	1137	1168	30			
1	C	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			
1	D	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



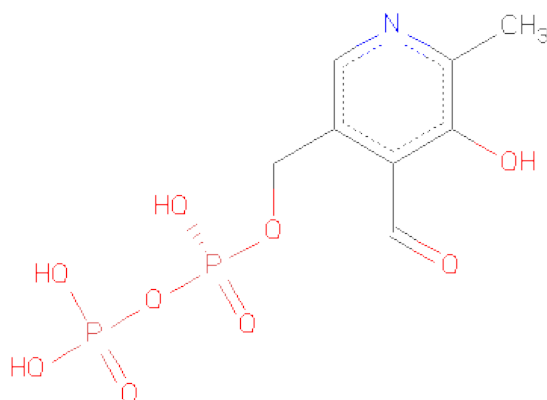
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (three-letter code: PDP) (formula:  $C_8H_{11}NO_9P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	B	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	C	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	D	1	Total	C	N	O	P	0	1
			38	16	2	16	4		

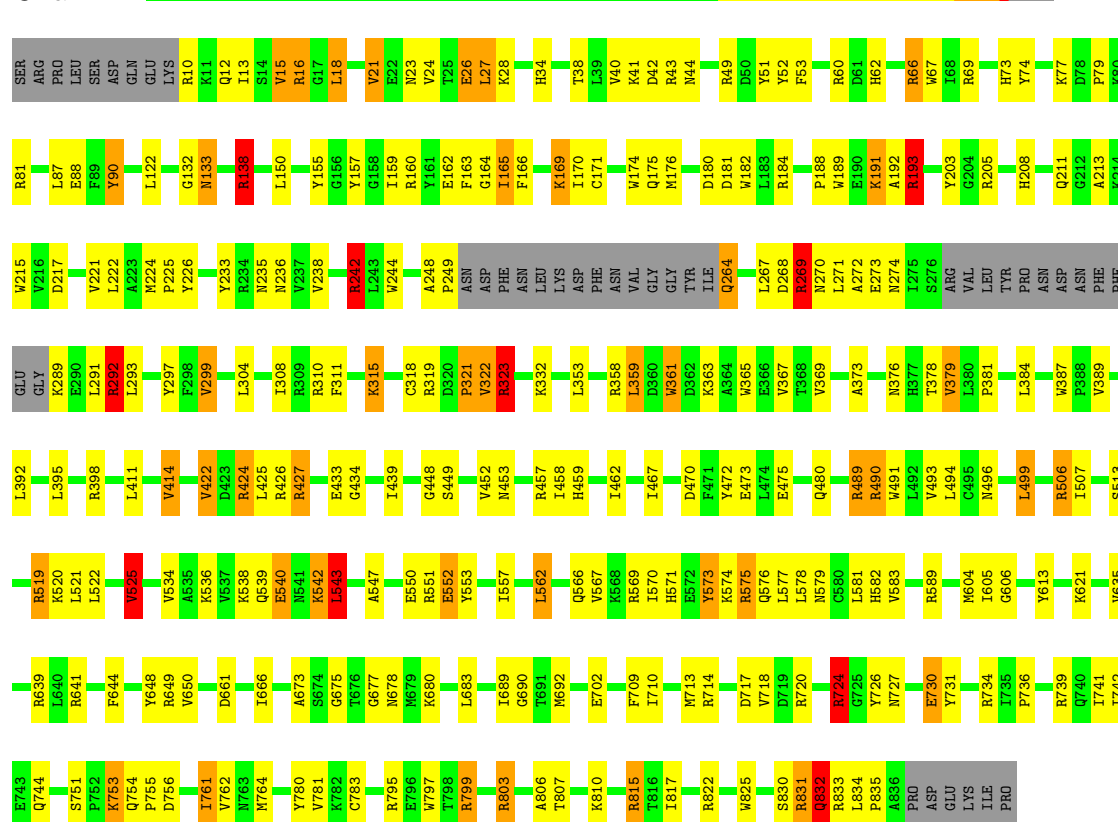
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

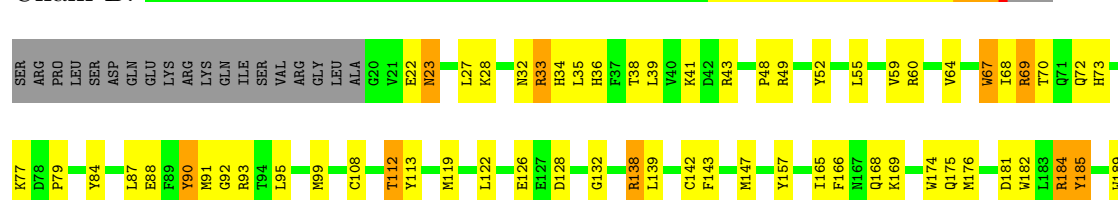
#### • Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain A:



#### • Molecule 1: GLYCOGEN PHOSPHORYLASE B

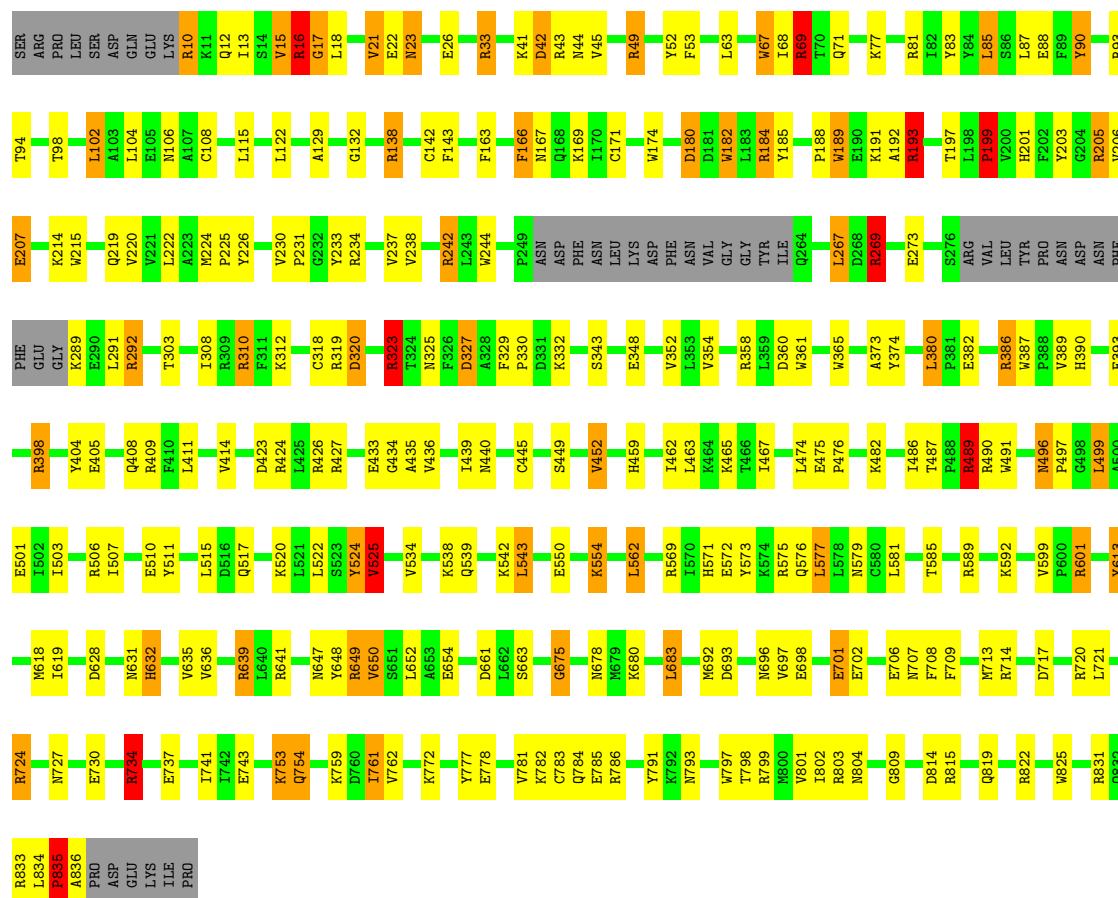
Chain B:





● Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90Å 209.90Å 123.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.87	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.87)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, PDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.85	0/6655	1.66	128/9001 (1.4%)
1	B	0.86	0/6577	1.63	129/8898 (1.4%)
1	C	0.82	0/6655	1.63	124/9001 (1.4%)
1	D	0.86	0/6655	1.65	132/9001 (1.5%)
All	All	0.85	0/26542	1.64	513/35901 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (513) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	ARG	NE-CZ-NH2	-14.56	113.02	120.30
1	D	601	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	A	639	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	B	489	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	D	138	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	D	193	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	B	815	ARG	NE-CZ-NH2	-12.00	114.30	120.30
1	A	242	ARG	NE-CZ-NH1	11.95	126.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	734	ARG	NE-CZ-NH1	11.89	126.24	120.30
1	A	815	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	D	138	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	D	69	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	B	193	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	D	575	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	D	323	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	C	310	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	C	575	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	B	831	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	C	457	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	815	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	D	424	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	B	323	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	D	601	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	182	TRP	CD1-CG-CD2	9.86	114.18	106.30
1	A	365	TRP	CD1-CG-CD2	9.84	114.17	106.30
1	C	724	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	C	815	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	649	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	C	613	TYR	CB-CG-CD2	-9.46	115.32	121.00
1	D	589	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	A	822	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	C	155	TYR	CB-CG-CD2	-9.21	115.47	121.00
1	B	815	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	A	799	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	D	639	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	D	831	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	D	589	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	B	409	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	A	780	TYR	CB-CG-CD2	-9.03	115.58	121.00
1	A	215	TRP	CD1-CG-CD2	9.02	113.51	106.30
1	A	189	TRP	CD1-CG-CD2	8.98	113.48	106.30
1	B	184	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	B	67	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	D	575	ARG	CB-CG-CD	-8.75	88.84	111.60
1	B	387	TRP	CD1-CG-CD2	8.73	113.29	106.30
1	C	67	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	A	720	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	C	361	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	C	182	TRP	CD1-CG-CD2	8.62	113.19	106.30
1	D	193	ARG	NE-CZ-NH1	8.61	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	365	TRP	CE2-CD2-CG	-8.55	100.46	107.30
1	C	387	TRP	CD1-CG-CD2	8.54	113.14	106.30
1	B	438	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	C	491	TRP	CD1-CG-CD2	8.47	113.07	106.30
1	C	174	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	B	215	TRP	CD1-CG-CD2	8.44	113.05	106.30
1	C	532	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	C	825	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	575	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	387	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	D	365	TRP	CD1-CG-CD2	8.38	113.01	106.30
1	A	138	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	B	575	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	310	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	C	113	TYR	CB-CG-CD1	-8.21	116.08	121.00
1	B	720	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	734	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	B	791	TYR	CB-CG-CD2	-8.14	116.12	121.00
1	C	189	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	A	489	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C	215	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	B	138	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	67	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	D	575	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	724	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	361	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	C	319	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	C	803	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	B	731	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	C	193	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	D	90	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	C	234	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	613	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	B	182	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	D	215	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	D	426	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	D	182	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	B	825	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	B	491	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	C	491	TRP	CE2-CD2-CG	-7.82	101.04	107.30
1	D	205	ARG	NE-CZ-NH2	-7.82	116.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	66	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	825	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A	244	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	575	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	C	387	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	D	310	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	D	184	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	189	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	B	387	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	C	398	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	C	556	HIS	CA-CB-CG	-7.67	100.57	113.60
1	B	506	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	365	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	C	562	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	67	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	489	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	D	613	TYR	CB-CG-CD2	-7.59	116.45	121.00
1	B	641	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	D	81	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	49	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	457	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	160	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	189	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	D	491	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	D	244	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	C	244	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	B	575	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	90	TYR	CB-CG-CD1	7.44	125.47	121.00
1	D	189	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	D	174	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	A	731	TYR	CB-CG-CD1	-7.41	116.56	121.00
1	B	244	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	D	174	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	60	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	292	ARG	CA-CB-CG	-7.36	97.22	113.40
1	C	182	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	365	TRP	CG-CD2-CE3	7.31	140.48	133.90
1	D	182	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	491	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	D	491	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	825	TRP	CE2-CD2-CG	-7.30	101.46	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	D	361	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	B	556	HIS	CA-CB-CG	-7.28	101.22	113.60
1	A	244	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	A	365	TRP	CB-CG-CD1	-7.26	117.56	127.00
1	B	234	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	174	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	B	641	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	215	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	233	TYR	CB-CG-CD1	-7.21	116.67	121.00
1	B	413	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	D	67	TRP	CD1-CG-CD2	7.21	112.06	106.30
1	D	777	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	C	457	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	C	90	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	C	52	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	A	81	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	160	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	D	171	CYS	CA-CB-SG	-7.18	101.08	114.00
1	B	27	LEU	CA-CB-CG	7.17	131.79	115.30
1	D	714	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	67	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	C	365	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	A	797	TRP	CD1-CG-CD2	7.13	112.01	106.30
1	C	189	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	C	361	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	D	69	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	825	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	D	386	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	825	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	215	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	C	67	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	B	831	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	797	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	B	60	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	174	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	C	413	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	639	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	323	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	16	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	491	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	B	189	TRP	CE2-CD2-CG	-6.96	101.73	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	TYR	CB-CG-CD2	-6.96	116.83	121.00
1	D	182	TRP	CG-CD2-CE3	6.96	140.16	133.90
1	C	797	TRP	CG-CD2-CE3	6.95	140.15	133.90
1	C	797	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	A	543	LEU	CA-CB-CG	6.93	131.23	115.30
1	A	835	PRO	N-CA-C	6.92	130.08	112.10
1	A	182	TRP	CD1-CG-CD2	6.91	111.83	106.30
1	B	292	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	404	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	D	189	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	B	786	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	361	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	D	67	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	B	215	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	A	66	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	540	GLU	CA-CB-CG	6.86	128.50	113.40
1	B	365	TRP	CD1-CG-CD2	6.86	111.78	106.30
1	D	825	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	797	TRP	CG-CD2-CE3	6.84	140.05	133.90
1	A	244	TRP	CG-CD2-CE3	6.84	140.05	133.90
1	A	639	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	714	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	491	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	B	184	ARG	CA-CB-CG	6.83	128.42	113.40
1	D	323	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	B	562	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	506	ARG	CA-CB-CG	-6.78	98.48	113.40
1	B	489	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	534	VAL	CG1-CB-CG2	-6.76	100.08	110.90
1	A	182	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	D	799	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	803	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	490	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	244	TRP	CE2-CD2-CG	-6.72	101.93	107.30
1	B	361	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	A	519	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	C	575	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	427	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	424	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	59	VAL	CG1-CB-CG2	-6.66	100.24	110.90
1	C	641	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	361	TRP	CE2-CD2-CG	-6.62	102.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	TRP	CD1-CG-CD2	6.62	111.60	106.30
1	C	292	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	215	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	D	207	GLU	CA-CB-CG	6.62	127.96	113.40
1	B	361	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	799	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	601	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	269	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	269	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	365	TRP	CD1-CG-CD2	6.58	111.57	106.30
1	A	174	TRP	CE2-CD2-CG	-6.57	102.04	107.30
1	D	33	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	D	244	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	D	825	TRP	CD1-CG-CD2	6.55	111.54	106.30
1	D	534	VAL	CG1-CB-CG2	-6.55	100.42	110.90
1	D	226	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	D	387	TRP	CE2-CD2-CG	-6.53	102.07	107.30
1	A	472	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	D	613	TYR	CB-CG-CD1	6.52	124.91	121.00
1	D	569	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	797	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	B	797	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	B	182	TRP	CG-CD1-NE1	-6.48	103.62	110.10
1	B	358	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	D	238	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	D	650	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	A	832	GLN	CA-CB-CG	6.46	127.60	113.40
1	A	203	TYR	CB-CG-CD2	-6.44	117.14	121.00
1	A	387	TRP	CG-CD2-CE3	6.43	139.69	133.90
1	D	426	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	822	ARG	CA-CB-CG	6.40	127.48	113.40
1	A	424	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	90	TYR	CA-CB-CG	6.36	125.49	113.40
1	C	160	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	365	TRP	CG-CD2-CE3	6.36	139.63	133.90
1	D	180	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	D	387	TRP	CD1-CG-CD2	6.35	111.38	106.30
1	D	365	TRP	CG-CD2-CE3	6.34	139.60	133.90
1	D	661	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	457	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	66	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	831	ARG	NE-CZ-NH1	6.32	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	770	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	422	VAL	CA-CB-CG1	-6.29	101.46	110.90
1	A	552	GLU	CA-CB-CG	6.29	127.24	113.40
1	B	310	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	138	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	365	TRP	CB-CG-CD1	-6.26	118.87	127.00
1	C	81	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	613	TYR	CB-CG-CD1	6.24	124.74	121.00
1	D	489	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	242	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	649	ARG	CG-CD-NE	-6.22	98.73	111.80
1	D	180	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	242	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	C	215	TRP	CG-CD1-NE1	-6.21	103.89	110.10
1	D	404	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	C	387	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	A	138	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	386	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	184	ARG	CG-CD-NE	6.19	124.80	111.80
1	B	309	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	174	TRP	CD1-CG-CD2	6.14	111.21	106.30
1	C	387	TRP	CG-CD2-CE3	6.14	139.42	133.90
1	D	489	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	562	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	438	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	511	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	C	714	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	739	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	310	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	16	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	D	797	TRP	CG-CD2-CE3	6.09	139.38	133.90
1	B	292	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	D	93	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	365	TRP	CG-CD1-NE1	-6.08	104.02	110.10
1	A	427	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	398	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	90	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	C	532	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	226	TYR	CB-CG-CD2	-6.06	117.37	121.00
1	C	797	TRP	CD1-CG-CD2	6.03	111.13	106.30
1	A	226	TYR	CB-CG-CD1	-6.02	117.39	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	797	TRP	CD1-CG-CD2	6.00	111.10	106.30
1	D	663	SER	CA-CB-OG	6.00	127.41	111.20
1	C	323	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	323	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	193	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	182	TRP	CG-CD2-CE3	5.96	139.27	133.90
1	C	525	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	A	387	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	A	292	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	60	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	720	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	42	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	234	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	215	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	B	797	TRP	CG-CD2-CE3	5.89	139.20	133.90
1	B	174	TRP	CB-CG-CD1	-5.89	119.35	127.00
1	D	292	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	D	85	LEU	CA-CB-CG	5.88	128.82	115.30
1	B	734	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	215	TRP	CG-CD2-CE3	5.88	139.19	133.90
1	B	692	MET	CG-SD-CE	5.88	109.60	100.20
1	C	182	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	D	734	ARG	CD-NE-CZ	5.85	131.79	123.60
1	C	67	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	A	835	PRO	CA-C-N	5.85	130.06	117.20
1	C	409	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	519	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	D	22	GLU	N-CA-C	-5.83	95.25	111.00
1	D	365	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	B	310	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	506	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	786	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	379	VAL	N-CA-C	-5.79	95.37	111.00
1	C	552	GLU	CA-C-N	5.79	129.94	117.20
1	D	163	PHE	N-CA-C	-5.78	95.39	111.00
1	A	797	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	B	193	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	506	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	292	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	244	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	825	TRP	CG-CD1-NE1	-5.76	104.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	525	VAL	CB-CA-C	-5.76	100.46	111.40
1	A	730	GLU	CA-CB-CG	-5.75	100.74	113.40
1	D	143	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	A	457	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	408	GLN	CA-CB-CG	5.75	126.06	113.40
1	A	358	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	C	489	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	299	VAL	CA-CB-CG2	-5.74	102.30	110.90
1	A	69	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	604	MET	CA-CB-CG	5.72	123.02	113.30
1	B	374	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	33	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	69	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	797	TRP	CD1-CG-CD2	5.71	110.87	106.30
1	D	424	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	482	LYS	N-CA-C	-5.70	95.60	111.00
1	A	189	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	D	822	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	569	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	67	TRP	CG-CD2-CE3	5.68	139.01	133.90
1	B	573	TYR	CA-CB-CG	5.67	124.17	113.40
1	C	90	TYR	CA-CB-CG	5.67	124.17	113.40
1	B	799	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	163	PHE	CA-C-N	5.66	127.52	116.20
1	C	424	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	43	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	393	GLU	CA-CB-CG	5.64	125.81	113.40
1	D	409	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	720	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	506	ARG	CA-CB-CG	-5.63	101.01	113.40
1	A	573	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	833	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	491	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	D	734	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	174	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	C	491	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	A	157	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	C	382	GLU	CA-C-N	-5.59	104.90	117.20
1	C	189	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	D	166	PHE	N-CA-C	5.58	126.06	111.00
1	C	361	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	A	268	ASP	CB-CA-C	-5.56	99.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	386	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	365	TRP	CB-CG-CD1	-5.54	119.80	127.00
1	B	814	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	205	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	833	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	491	TRP	CB-CG-CD1	-5.50	119.84	127.00
1	A	13	ILE	N-CA-C	-5.50	96.16	111.00
1	A	427	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	825	TRP	CG-CD2-CE3	5.48	138.84	133.90
1	A	16	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	365	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	B	189	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	C	390	HIS	CA-CB-CG	5.47	122.91	113.60
1	D	524	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	D	205	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	714	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	409	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	803	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	67	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	B	321	PRO	N-CA-C	5.45	126.26	112.10
1	C	641	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	720	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	519	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	269	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	354	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	B	22	GLU	N-CA-C	-5.42	96.36	111.00
1	B	491	TRP	CG-CD2-CE3	5.42	138.77	133.90
1	A	550	GLU	CA-CB-CG	5.41	125.31	113.40
1	B	182	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	A	299	VAL	CA-CB-CG1	5.40	119.00	110.90
1	B	49	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	51	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	B	185	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	D	215	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	D	814	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	323	ARG	CA-CB-CG	-5.38	101.56	113.40
1	C	266	VAL	N-CA-C	-5.38	96.47	111.00
1	B	157	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	553	TYR	CA-CB-CG	5.37	123.60	113.40
1	C	825	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	D	649	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	491	TRP	CG-CD1-NE1	-5.36	104.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	TRP	CB-CG-CD1	-5.35	120.04	127.00
1	D	724	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	69	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	84	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	358	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	797	TRP	CB-CG-CD1	-5.32	120.09	127.00
1	A	825	TRP	CB-CG-CD1	-5.31	120.09	127.00
1	A	42	ASP	CA-CB-CG	5.31	125.08	113.40
1	B	322	VAL	CA-CB-CG2	-5.31	102.94	110.90
1	B	387	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	B	23	ASN	N-CA-C	-5.30	96.68	111.00
1	A	67	TRP	CB-CG-CD1	-5.28	120.13	127.00
1	C	174	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	C	424	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	436	VAL	CA-CB-CG1	-5.28	102.98	110.90
1	C	78	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	613	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	B	372	CYS	CA-CB-SG	-5.26	104.53	114.00
1	B	519	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	234	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	215	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	C	237	VAL	CA-CB-CG2	-5.25	103.03	110.90
1	C	413	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	182	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	C	93	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	491	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	C	603	VAL	CG1-CB-CG2	-5.22	102.55	110.90
1	D	182	TRP	NE1-CE2-CZ2	-5.22	124.66	130.40
1	A	49	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	525	VAL	CB-CA-C	-5.21	101.50	111.40
1	C	636	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	D	102	LEU	CA-CB-CG	5.21	127.27	115.30
1	D	835	PRO	N-CA-C	5.20	125.62	112.10
1	B	381	PRO	CA-C-N	-5.20	105.76	117.20
1	D	361	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	A	69	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	613	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	322	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	B	491	TRP	CB-CG-CD1	-5.17	120.27	127.00
1	D	613	TYR	N-CA-C	-5.17	97.03	111.00
1	D	562	LEU	CA-CB-CG	5.17	127.18	115.30
1	C	161	TYR	CB-CG-CD2	-5.15	117.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	575	ARG	CB-CG-CD	-5.14	98.23	111.60
1	A	426	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	836	ALA	N-CA-CB	5.13	117.29	110.10
1	B	244	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	A	552	GLU	N-CA-C	-5.12	97.17	111.00
1	B	791	TYR	CB-CG-CD1	5.12	124.07	121.00
1	B	822	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	797	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	C	551	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	43	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	242	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	701	GLU	CA-CB-CG	5.09	124.60	113.40
1	C	33	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	759	LYS	CA-CB-CG	-5.09	102.20	113.40
1	D	727	ASN	N-CA-C	-5.09	97.26	111.00
1	D	632	HIS	CA-CB-CG	-5.08	104.95	113.60
1	C	822	ARG	N-CA-CB	-5.08	101.45	110.60
1	D	825	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	C	84	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	142	CYS	CA-CB-SG	5.06	123.11	114.00
1	B	60	ARG	CB-CG-CD	-5.05	98.46	111.60
1	C	556	HIS	CA-C-N	-5.05	106.09	117.20
1	C	189	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	B	27	LEU	CB-CA-C	-5.04	100.62	110.20
1	A	422	VAL	CB-CA-C	-5.04	101.82	111.40
1	B	835	PRO	N-CA-CB	-5.04	97.06	102.60
1	C	490	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	155	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	825	TRP	CG-CD1-NE1	-5.03	105.08	110.10
1	C	215	TRP	N-CA-C	-5.03	97.43	111.00
1	D	108	CYS	CA-CB-SG	-5.03	104.95	114.00
1	A	553	TYR	CA-CB-CG	5.02	122.94	113.40
1	B	43	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	181	ASP	N-CA-CB	5.02	119.63	110.60
1	B	421	ASP	N-CA-C	5.01	124.53	111.00
1	D	801	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	B	780	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	C	113	TYR	CG-CD2-CE2	-5.01	117.29	121.30
1	D	16	ARG	N-CA-C	5.01	124.52	111.00
1	D	585	THR	CA-CB-CG2	5.01	119.41	112.40
1	D	361	TRP	CG-CD1-NE1	-5.00	105.09	110.10
1	D	803	ARG	NE-CZ-NH1	5.00	122.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	780	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	TYR	Sidechain
1	A	52	TYR	Sidechain
1	B	52	TYR	Sidechain
1	B	834	LEU	Peptide
1	C	52	TYR	Sidechain
1	C	791	TYR	Sidechain
1	D	511	TYR	Sidechain
1	D	524	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6512	0	6484	115	0
1	B	6434	0	6393	121	0
1	C	6512	0	6484	131	0
1	D	6512	0	6484	113	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	38	0	14	0	0
3	B	38	0	14	1	0
3	C	38	0	13	0	0
3	D	38	0	14	0	0
All	All	26214	0	25948	468	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (468) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.63	0.81
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.61	0.79
1:C:549:LEU:HD12	1:C:557:ILE:HD13	1.65	0.79
1:B:325:ASN:HD21	1:B:327:ASP:HB2	1.52	0.75
1:C:88:GLU:HB2	1:C:132:GLY:HA2	1.68	0.75
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.67	0.74
1:B:201:HIS:CD2	1:B:220:VAL:HG22	2.23	0.74
1:A:496:ASN:OD1	1:A:499:LEU:HB2	1.89	0.73
1:B:235:ASN:HA	1:B:833:ARG:HG2	1.69	0.72
1:B:753:LYS:HG2	1:B:754:GLN:HG3	1.72	0.70
1:A:582:HIS:HD2	1:A:781:VAL:HG22	1.56	0.70
1:C:122:LEU:HA	1:C:125:ILE:HD12	1.72	0.70
1:D:237:VAL:HG22	1:D:834:LEU:HD22	1.75	0.68
1:C:578:LEU:HD22	1:C:780:TYR:CD2	2.28	0.68
1:C:532:ARG:HH11	1:C:532:ARG:HB3	1.56	0.68
1:B:290:GLU:HG3	1:B:391:LEU:HD11	1.75	0.68
1:C:709:PHE:HB3	1:C:783:CYS:SG	2.34	0.68
1:D:459:HIS:HA	1:D:462:ILE:HD12	1.75	0.67
1:B:380:LEU:HB3	1:B:382:GLU:HB2	1.77	0.67
1:C:539:GLN:NE2	1:C:543:LEU:HD22	2.09	0.67
1:A:754:GLN:HE22	1:D:434:GLY:HA3	1.60	0.66
1:A:379:VAL:HG22	1:A:673:ALA:HB2	1.78	0.66
1:A:222:LEU:HG	1:A:249:PRO:HB3	1.78	0.66
1:C:21:VAL:HG21	1:C:23:ASN:ND2	2.11	0.66
1:C:82:ILE:HD11	1:C:827:VAL:HG21	1.78	0.66
1:C:175:GLN:NE2	1:C:617:LYS:HE2	2.12	0.65
1:C:577:LEU:HD11	1:C:761:ILE:HD12	1.77	0.65
1:B:33:ARG:HG2	1:B:33:ARG:HH11	1.61	0.65
1:D:730:GLU:O	1:D:734:ARG:HG2	1.97	0.64
1:B:227:ASP:OD1	1:B:242:ARG:HD3	1.98	0.64
1:D:269:ARG:HH11	1:D:269:ARG:HB2	1.63	0.64
1:B:225:PRO:HG3	1:B:244:TRP:CZ3	2.33	0.63
1:C:93:ARG:HD2	1:C:126:GLU:HB3	1.79	0.63
1:A:753:LYS:HG2	1:A:754:GLN:HG2	1.81	0.63
1:D:539:GLN:HE21	1:D:543:LEU:HD22	1.64	0.63
1:C:629:VAL:HG21	1:C:750:PHE:HD1	1.64	0.62
1:C:546:ALA:HA	1:C:557:ILE:HD11	1.81	0.62
1:D:33:ARG:HH11	1:D:33:ARG:HG2	1.65	0.62
1:C:547:ALA:O	1:C:551:ARG:HG2	2.00	0.61
1:A:677:GLY:HA2	1:A:680:LYS:HE2	1.82	0.61
1:B:35:LEU:HD12	1:B:39:LEU:HD12	1.82	0.61
1:C:599:VAL:HG11	1:C:791:TYR:HD2	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:613:TYR:CD2	1:B:616:ALA:HB2	2.36	0.61
1:A:539:GLN:O	1:A:543:LEU:HD22	2.01	0.61
1:B:201:HIS:HD2	1:B:220:VAL:HG22	1.64	0.60
1:B:225:PRO:HB3	1:B:242:ARG:HD2	1.82	0.60
1:A:724:ARG:NH1	1:A:726:TYR:HA	2.16	0.60
1:C:648:TYR:HA	1:C:652:LEU:HD23	1.83	0.60
1:A:795:ARG:O	1:A:799:ARG:HG3	2.02	0.60
1:C:24:VAL:HG13	1:C:111:ALA:HA	1.84	0.60
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.83	0.59
1:C:810:LYS:O	1:C:815:ARG:HD3	2.02	0.59
1:C:10:ARG:N	1:D:115:LEU:O	2.36	0.59
1:D:323:ARG:HH12	1:D:332:LYS:HE3	1.66	0.59
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.66	0.59
1:D:753:LYS:HG2	1:D:754:GLN:HG3	1.85	0.58
1:A:181:ASP:HB3	1:A:184:ARG:NH2	2.18	0.58
1:D:692:MET:SD	1:D:697:VAL:HG22	2.43	0.58
1:D:538:LYS:O	1:D:542:LYS:HG3	2.03	0.58
1:C:343:SER:HB3	1:C:445:CYS:SG	2.43	0.58
1:A:724:ARG:HH22	1:A:727:ASN:H	1.51	0.58
1:D:192:ALA:HB1	1:D:224:MET:HE1	1.86	0.58
1:C:235:ASN:HA	1:C:833:ARG:HG3	1.85	0.58
1:C:690:GLY:O	1:C:710:ILE:HA	2.04	0.58
1:B:384:LEU:HB2	1:B:386:ARG:NH1	2.19	0.58
1:B:112:THR:HG22	1:B:113:TYR:HD1	1.69	0.57
1:B:719:ASP:O	1:B:723:GLN:HG3	2.04	0.57
1:A:414:VAL:HG22	1:A:425:LEU:HD23	1.86	0.57
1:D:21:VAL:HB	1:D:23:ASN:HB3	1.85	0.57
1:A:248:ALA:HB2	1:A:269:ARG:HA	1.85	0.57
1:D:325:ASN:HD21	1:D:327:ASP:HB2	1.69	0.57
1:D:88:GLU:HB2	1:D:132:GLY:HA2	1.86	0.57
1:B:224:MET:HB2	1:B:247:LYS:HE2	1.86	0.57
1:B:612:GLY:H	1:B:617:LYS:HZ2	1.53	0.57
1:D:510:GLU:HB2	1:D:517:GLN:HE22	1.70	0.57
1:C:792:LYS:O	1:C:794:PRO:HD3	2.05	0.57
1:B:184:ARG:HD2	1:B:185:TYR:CE2	2.40	0.56
1:B:205:ARG:HG3	1:B:216:VAL:HG23	1.87	0.56
1:C:613:TYR:CD2	1:C:616:ALA:HB2	2.40	0.56
1:C:293:LEU:HD21	1:C:392:LEU:HD23	1.86	0.56
1:B:668:THR:OG1	1:B:771:PHE:HB3	2.05	0.56
1:A:73:HIS:NE2	1:A:77:LYS:HD3	2.20	0.56
1:D:53:PHE:HE1	1:D:188:PRO:HD3	1.69	0.56
1:B:384:LEU:HB2	1:B:386:ARG:HH12	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:ARG:NH1	1:A:332:LYS:HE3	2.20	0.56
1:C:463:LEU:HD23	1:C:467:ILE:HD12	1.88	0.56
1:D:462:ILE:HG22	1:D:467:ILE:HG13	1.87	0.56
1:A:424:ARG:HG3	1:A:427:ARG:HH21	1.71	0.56
1:C:578:LEU:HD21	1:C:777:TYR:HA	1.87	0.55
1:B:636:VAL:O	1:B:639:ARG:HD3	2.07	0.55
1:C:455:VAL:HG23	1:C:674:SER:HB2	1.88	0.55
1:B:453:ASN:ND2	1:B:482:LYS:HB2	2.21	0.55
1:B:321:PRO:O	1:B:322:VAL:HG12	2.07	0.55
1:D:318:CYS:SG	1:D:320:ASP:HB2	2.47	0.55
1:D:636:VAL:O	1:D:639:ARG:HD3	2.06	0.55
1:C:636:VAL:O	1:C:639:ARG:HD3	2.07	0.55
1:D:781:VAL:O	1:D:785:GLU:HG3	2.06	0.55
1:C:269:ARG:HB2	1:C:269:ARG:HH11	1.72	0.55
1:D:753:LYS:HD2	1:D:753:LYS:H	1.71	0.55
1:C:726:TYR:HE1	1:C:775:ALA:HB2	1.72	0.55
1:D:486:ILE:HD13	1:D:680:LYS:HG3	1.87	0.55
1:D:380:LEU:HD13	1:D:382:GLU:HB2	1.88	0.55
1:C:677:GLY:HA2	1:C:680:LYS:HD3	1.89	0.55
1:A:571:HIS:HD2	1:A:573:TYR:H	1.53	0.55
1:D:343:SER:HB3	1:D:445:CYS:SG	2.46	0.54
1:B:734:ARG:N	1:B:734:ARG:HD2	2.22	0.54
1:B:502:ILE:HA	1:B:505:GLU:HG2	1.89	0.54
1:C:37:PHE:HE2	1:D:18:LEU:HB3	1.73	0.54
1:D:203:TYR:HD2	1:D:219:GLN:HG2	1.72	0.54
1:A:353:LEU:O	1:A:359:LEU:HB2	2.07	0.54
1:B:622:LEU:HD22	1:B:761:ILE:HD13	1.89	0.54
1:B:143:PHE:O	1:B:147:MET:HG3	2.08	0.54
1:A:458:ILE:HG22	1:A:462:ILE:HD11	1.89	0.54
1:B:32:ASN:O	1:B:36:HIS:HD2	1.90	0.54
1:B:237:VAL:HG22	1:B:834:LEU:HD22	1.89	0.54
1:D:42:ASP:HB2	1:D:45:VAL:HG22	1.89	0.54
1:D:325:ASN:ND2	1:D:327:ASP:HB2	2.22	0.54
1:C:436:VAL:HG12	1:C:438:ARG:HG3	1.90	0.54
1:A:88:GLU:HB2	1:A:132:GLY:HA2	1.90	0.54
1:C:575:ARG:HH22	1:C:776:ASP:HB2	1.72	0.54
1:A:74:TYR:O	1:A:79:PRO:HD2	2.08	0.54
1:D:102:LEU:HD23	1:D:104:LEU:HD12	1.90	0.54
1:B:93:ARG:HD3	1:B:126:GLU:O	2.08	0.54
1:B:108:CYS:O	1:B:112:THR:HB	2.08	0.53
1:D:650:VAL:O	1:D:654:GLU:HG3	2.07	0.53
1:C:115:LEU:HD23	1:D:12:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:24:VAL:O	1:C:28:LYS:HG3	2.08	0.53
1:C:169:LYS:HB2	1:C:169:LYS:NZ	2.24	0.53
1:A:133:ASN:OD1	1:A:165:ILE:HG12	2.09	0.53
1:B:707:ASN:HA	1:B:800:MET:HE2	1.91	0.53
1:B:721:LEU:HD23	1:B:772:LYS:HD3	1.90	0.53
1:C:41:LYS:HG3	1:C:45:VAL:HG23	1.90	0.53
1:A:170:ILE:HD13	1:A:175:GLN:HA	1.91	0.53
1:C:413:ARG:NH1	1:C:474:LEU:HD21	2.24	0.53
1:C:422:VAL:HA	1:C:425:LEU:HD12	1.90	0.53
1:C:378:THR:HG21	1:C:384:LEU:HD21	1.90	0.53
1:C:271:LEU:HA	1:C:274:ASN:HB2	1.91	0.53
1:A:293:LEU:HD23	1:A:395:LEU:HD23	1.91	0.53
1:D:380:LEU:CD1	1:D:382:GLU:HB2	2.38	0.53
1:B:619:ILE:O	1:B:623:ILE:HG13	2.08	0.52
1:D:184:ARG:HD2	1:D:185:TYR:CE2	2.44	0.52
1:C:142:CYS:SG	1:C:487:THR:HG22	2.49	0.52
1:A:567:VAL:HA	1:A:606:GLY:O	2.09	0.52
1:C:205:ARG:HG3	1:C:216:VAL:HG23	1.91	0.52
1:A:293:LEU:HD21	1:A:392:LEU:HD23	1.92	0.52
1:D:63:LEU:HD11	1:D:231:PRO:HD3	1.90	0.52
1:C:89:PHE:O	1:C:131:LEU:HB2	2.10	0.52
1:D:713:MET:HB3	1:D:717:ASP:HB2	1.92	0.52
1:B:70:THR:O	1:B:73:HIS:HB3	2.09	0.52
1:C:32:ASN:OD1	1:D:13:ILE:HA	2.09	0.52
1:C:532:ARG:HB3	1:C:532:ARG:NH1	2.24	0.52
1:A:181:ASP:HB3	1:A:184:ARG:HH21	1.74	0.52
1:B:225:PRO:HG3	1:B:244:TRP:HZ3	1.72	0.51
1:A:323:ARG:HH12	1:A:332:LYS:HE3	1.75	0.51
1:A:159:ILE:HG13	1:A:299:VAL:HG23	1.92	0.51
1:D:289:LYS:HD2	1:D:291:LEU:HD13	1.92	0.51
1:D:486:ILE:HD11	1:D:683:LEU:HD12	1.93	0.51
1:B:577:LEU:HD11	1:B:761:ILE:HD12	1.91	0.51
1:C:736:PRO:HG3	1:C:739:ARG:HH22	1.76	0.51
1:D:737:GLU:O	1:D:741:ILE:HG13	2.11	0.51
1:B:112:THR:HG22	1:B:113:TYR:CD1	2.46	0.51
1:D:577:LEU:HD13	1:D:619:ILE:HG12	1.93	0.51
1:C:583:VAL:HG11	1:C:603:VAL:HG11	1.92	0.51
1:C:522:LEU:O	1:C:525:VAL:HG23	2.10	0.51
1:A:736:PRO:HG3	1:A:739:ARG:NH2	2.26	0.51
1:C:10:ARG:HD2	1:C:10:ARG:N	2.26	0.51
1:D:499:LEU:HD22	1:D:503:ILE:HD11	1.93	0.51
1:C:442:ALA:O	1:C:446:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:815:ARG:O	1:D:819:GLN:HG3	2.11	0.50
1:A:742:ILE:HG23	1:A:762:VAL:HG13	1.92	0.50
1:B:578:LEU:HD22	1:B:780:TYR:CD2	2.47	0.50
1:D:386:ARG:HA	1:D:439:ILE:O	2.11	0.50
1:C:631:ASN:OD1	1:C:641:ARG:HA	2.11	0.50
1:C:157:TYR:CE2	1:C:242:ARG:HG2	2.45	0.50
1:B:612:GLY:H	1:B:617:LYS:NZ	2.09	0.50
1:C:580:CYS:HA	1:C:583:VAL:HG22	1.93	0.50
1:B:636:VAL:O	1:B:639:ARG:HB2	2.12	0.50
1:A:730:GLU:O	1:A:734:ARG:HG2	2.11	0.50
1:B:34:HIS:O	1:B:38:THR:HB	2.12	0.50
1:A:53:PHE:CE1	1:A:188:PRO:HG3	2.47	0.50
1:B:631:ASN:OD1	1:B:641:ARG:HA	2.12	0.50
1:A:235:ASN:O	1:A:236:ASN:HB2	2.10	0.50
1:C:622:LEU:HD22	1:C:761:ILE:HD11	1.94	0.50
1:D:42:ASP:HB3	1:D:44:ASN:H	1.76	0.50
1:A:605:ILE:O	1:A:644:PHE:HA	2.11	0.50
1:C:182:TRP:CE2	1:C:183:LEU:HG	2.47	0.50
1:A:689:ILE:HA	1:A:709:PHE:HB2	1.93	0.50
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.92	0.50
1:C:42:ASP:HB3	1:C:44:ASN:H	1.77	0.50
1:B:465:LYS:HD2	1:B:465:LYS:N	2.27	0.50
1:C:413:ARG:HH12	1:C:474:LEU:HD21	1.77	0.50
1:C:289:LYS:HD3	1:C:291:LEU:H	1.76	0.50
1:C:734:ARG:HH11	1:C:734:ARG:HB3	1.77	0.49
1:B:587:TYR:O	1:B:591:LYS:HG2	2.12	0.49
1:D:386:ARG:HG2	1:D:440:ASN:HD22	1.77	0.49
1:A:536:LYS:O	1:A:540:GLU:HG3	2.12	0.49
1:C:730:GLU:HB3	1:C:734:ARG:NH2	2.28	0.49
1:B:822:ARG:HD2	1:B:828:GLU:OE1	2.12	0.49
1:D:522:LEU:O	1:D:525:VAL:HG22	2.11	0.49
1:C:730:GLU:HB3	1:C:734:ARG:HH21	1.76	0.49
1:A:690:GLY:O	1:A:710:ILE:HA	2.12	0.49
1:B:68:ILE:O	1:B:72:GLN:HG3	2.13	0.49
1:A:62:HIS:HB3	1:A:66:ARG:HH21	1.78	0.49
1:D:323:ARG:NH1	1:D:332:LYS:HE3	2.28	0.49
1:C:269:ARG:HB2	1:C:269:ARG:NH1	2.28	0.49
1:D:308:ILE:HG22	1:D:312:LYS:HE2	1.94	0.49
1:D:197:THR:CG2	1:D:222:LEU:HB3	2.42	0.49
1:C:171:CYS:SG	1:C:176:MET:SD	3.11	0.49
1:A:830:SER:OG	1:A:832:GLN:HG3	2.12	0.49
1:A:318:CYS:SG	1:A:319:ARG:N	2.87	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:486:ILE:HD13	1:C:680:LYS:HG3	1.95	0.48
1:A:44:ASN:HD21	1:B:72:GLN:NE2	2.12	0.48
1:A:21:VAL:HG23	1:A:26:GLU:HG2	1.94	0.48
1:D:129:ALA:HA	1:D:182:TRP:CE3	2.48	0.48
1:D:647:ASN:HB3	1:D:649:ARG:HH21	1.79	0.48
1:A:24:VAL:HG12	1:A:28:LYS:HE2	1.94	0.48
1:D:709:PHE:HB3	1:D:783:CYS:SG	2.53	0.48
1:A:12:GLN:HE22	1:B:28:LYS:NZ	2.10	0.48
1:A:761:ILE:HG13	1:A:762:VAL:N	2.28	0.48
1:D:423:ASP:O	1:D:427:ARG:HG3	2.13	0.48
1:B:767:HIS:O	1:B:768:HIS:ND1	2.47	0.48
1:D:373:ALA:HA	1:D:449:SER:HB3	1.94	0.48
1:A:311:PHE:CZ	1:A:323:ARG:HD2	2.49	0.48
1:A:832:GLN:HE22	1:A:834:LEU:HD13	1.79	0.48
1:C:726:TYR:OH	1:C:774:PHE:HB2	2.14	0.48
1:A:163:PHE:HA	1:A:180:ASP:O	2.13	0.48
1:C:235:ASN:O	1:C:236:ASN:HB2	2.14	0.48
1:C:597:PHE:HE2	1:C:792:LYS:HD3	1.79	0.48
1:D:49:ARG:HG2	1:D:53:PHE:CE2	2.49	0.47
1:D:10:ARG:HA	1:D:13:ILE:HD12	1.96	0.47
1:D:85:LEU:HD13	1:D:303:THR:HG21	1.96	0.47
1:B:538:LYS:HG3	1:B:542:LYS:HD3	1.96	0.47
1:B:201:HIS:HB3	1:B:218:THR:HB	1.97	0.47
1:C:732:TYR:HA	1:C:738:LEU:HD23	1.95	0.47
1:B:325:ASN:ND2	1:B:327:ASP:HB2	2.24	0.47
1:C:175:GLN:HE21	1:C:617:LYS:HE2	1.78	0.47
1:C:594:PRO:HB3	1:C:635:VAL:HG23	1.96	0.47
1:C:237:VAL:HG22	1:C:834:LEU:HD22	1.97	0.47
1:B:378:THR:O	1:B:459:HIS:NE2	2.48	0.47
1:B:67:TRP:HD1	1:B:238:VAL:HG12	1.80	0.47
1:B:93:ARG:HD2	1:B:126:GLU:HB3	1.96	0.47
1:D:94:THR:HG22	1:D:98:THR:OG1	2.15	0.47
1:B:799:ARG:O	1:B:803:ARG:HG3	2.14	0.47
1:B:800:MET:HA	1:B:803:ARG:NH1	2.30	0.47
1:C:633:ASP:OD2	1:C:635:VAL:HG13	2.15	0.47
1:D:675:GLY:O	1:D:678:ASN:HB2	2.15	0.47
1:C:90:TYR:HD2	1:C:138:ARG:HG2	1.79	0.47
1:B:486:ILE:HD13	1:B:680:LYS:HG3	1.97	0.47
1:C:59:VAL:HG13	1:C:104:LEU:HD12	1.96	0.47
1:A:373:ALA:HA	1:A:449:SER:HB3	1.97	0.47
1:B:533:ASP:O	1:B:537:VAL:HG23	2.14	0.47
1:A:378:THR:O	1:A:459:HIS:NE2	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:MET:HE2	1:B:241:MET:SD	2.55	0.47
1:A:810:LYS:O	1:A:815:ARG:HD3	2.13	0.47
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.97	0.47
1:B:566:GLN:NE2	1:B:576:GLN:HA	2.30	0.47
1:D:83:TYR:HE2	1:D:310:ARG:HH21	1.63	0.47
1:C:337:LEU:HD21	1:C:345:ALA:HB3	1.97	0.47
1:A:569:ARG:O	1:A:574:LYS:HG3	2.15	0.47
1:D:329:PHE:HB3	1:D:330:PRO:HD3	1.96	0.47
1:C:793:ASN:OD1	1:C:796:GLU:HG2	2.15	0.46
1:D:507:ILE:HG21	1:D:520:LYS:HB3	1.95	0.46
1:C:525:VAL:HG12	1:C:799:ARG:NH1	2.30	0.46
1:C:143:PHE:O	1:C:147:MET:HG3	2.15	0.46
1:D:206:VAL:HA	1:D:214:LYS:O	2.15	0.46
1:C:407:ASN:ND2	1:C:411:LEU:HD22	2.30	0.46
1:B:397:PRO:O	1:B:401:GLN:HG3	2.15	0.46
1:B:717:ASP:HA	1:B:720:ARG:HH11	1.81	0.46
1:B:721:LEU:HD21	1:B:726:TYR:HD1	1.80	0.46
1:D:507:ILE:HG21	1:D:520:LYS:CB	2.46	0.46
1:D:15:VAL:O	1:D:17:GLY:N	2.47	0.46
1:C:622:LEU:HD22	1:C:761:ILE:CD1	2.46	0.46
1:B:721:LEU:HD21	1:B:726:TYR:CD1	2.49	0.46
1:B:330:PRO:HD3	1:B:367:VAL:HG13	1.96	0.46
1:B:677:GLY:HA2	1:B:680:LYS:HD3	1.96	0.46
1:B:386:ARG:HA	1:B:439:ILE:O	2.15	0.46
1:A:44:ASN:HD21	1:B:72:GLN:HE21	1.63	0.46
1:A:434:GLY:HA2	1:D:754:GLN:HE22	1.81	0.46
1:B:113:TYR:HE1	1:B:119:MET:H	1.62	0.46
1:B:543:LEU:HD12	1:B:559:PRO:HB2	1.98	0.46
1:C:160:ARG:HG3	1:C:243:LEU:HD12	1.97	0.46
1:B:95:LEU:HG	1:B:99:MET:HE2	1.98	0.46
1:B:431:VAL:HG11	1:B:437:LYS:HE3	1.98	0.46
1:D:693:ASP:O	1:D:696:ASN:HB2	2.16	0.46
1:A:538:LYS:O	1:A:542:LYS:HG3	2.16	0.46
1:B:165:ILE:HD12	1:B:165:ILE:HA	1.74	0.46
1:C:629:VAL:HG21	1:C:750:PHE:CD1	2.47	0.45
1:C:531:ILE:O	1:C:798:THR:HG21	2.15	0.45
1:D:192:ALA:HB1	1:D:224:MET:CE	2.46	0.45
1:A:208:HIS:HA	1:A:213:ALA:HA	1.99	0.45
1:A:66:ARG:HB3	1:A:238:VAL:HG21	1.98	0.45
1:A:221:VAL:HG13	1:A:272:ALA:HB1	1.98	0.45
1:A:575:ARG:HD3	1:A:666:ILE:O	2.16	0.45
1:C:349:LEU:HD23	1:C:368:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:648:TYR:HA	1:D:652:LEU:HD23	1.99	0.45
1:C:225:PRO:HB3	1:C:244:TRP:CZ3	2.51	0.45
1:C:168:GLN:HG3	1:C:175:GLN:HG3	1.98	0.45
1:A:73:HIS:CE1	1:A:77:LYS:HD3	2.51	0.45
1:A:264:GLN:HG3	1:A:267:LEU:HG	1.97	0.45
1:C:11:LYS:HA	1:D:43:ARG:CZ	2.47	0.45
1:D:515:LEU:HG	1:D:809:GLY:HA2	1.98	0.45
1:C:464:LYS:HD3	1:C:472:TYR:CE1	2.51	0.45
1:C:293:LEU:HD21	1:C:392:LEU:CD2	2.47	0.45
1:D:98:THR:O	1:D:102:LEU:HB2	2.16	0.45
1:A:567:VAL:HB	1:A:648:TYR:CZ	2.51	0.45
1:B:571:HIS:HD2	1:B:573:TYR:H	1.64	0.45
1:A:389:VAL:HG12	1:A:439:ILE:HG12	1.99	0.45
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.81	0.45
1:C:566:GLN:O	1:C:605:ILE:HA	2.17	0.45
1:B:648:TYR:HA	1:B:652:LEU:HD23	1.98	0.45
1:D:721:LEU:HD23	1:D:772:LYS:HD3	1.99	0.45
1:A:525:VAL:O	1:A:799:ARG:HD2	2.16	0.45
1:A:164:GLY:N	1:A:180:ASP:HB3	2.32	0.45
1:C:192:ALA:HB2	1:C:226:TYR:CE2	2.52	0.45
1:B:786:ARG:HH11	1:B:786:ARG:HG3	1.82	0.45
1:D:463:LEU:HD23	1:D:467:ILE:HD12	1.98	0.45
1:B:720:ARG:HA	1:B:723:GLN:OE1	2.17	0.45
1:C:566:GLN:HE22	1:C:576:GLN:HA	1.82	0.45
1:D:67:TRP:HE3	1:D:68:ILE:HG13	1.82	0.45
1:B:546:ALA:HA	1:B:557:ILE:HD11	1.98	0.45
1:A:23:ASN:O	1:A:27:LEU:HD22	2.17	0.44
1:D:601:ARG:NH2	1:D:784:GLN:OE1	2.50	0.44
1:A:289:LYS:HG3	1:A:291:LEU:H	1.82	0.44
1:B:573:TYR:CZ	1:B:574:LYS:HE2	2.52	0.44
1:A:267:LEU:O	1:A:271:LEU:HG	2.17	0.44
1:A:192:ALA:HB1	1:A:224:MET:CE	2.47	0.44
1:C:550:GLU:HB2	1:C:556:HIS:NE2	2.33	0.44
1:B:611:PRO:HA	1:B:617:LYS:HZ1	1.82	0.44
1:C:376:ASN:OD1	1:C:378:THR:HG22	2.16	0.44
1:A:315:LYS:HB3	1:A:318:CYS:HB3	1.99	0.44
1:B:571:HIS:CD2	1:B:572:GLU:N	2.85	0.44
1:D:761:ILE:HG13	1:D:762:VAL:N	2.32	0.44
1:A:507:ILE:HG21	1:A:520:LYS:HB2	1.99	0.44
1:C:616:ALA:HA	1:C:619:ILE:HD12	1.99	0.44
1:A:169:LYS:HG3	1:A:171:CYS:SG	2.56	0.44
1:C:353:LEU:HD13	1:C:359:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:736:PRO:HG3	1:A:739:ARG:HH22	1.80	0.44
1:D:599:VAL:HG11	1:D:791:TYR:HD2	1.81	0.44
1:D:707:ASN:HB3	1:D:804:ASN:HD21	1.82	0.44
1:C:48:PRO:HB3	1:C:125:ILE:HD11	2.00	0.44
1:D:698:GLU:HA	1:D:701:GLU:HG3	2.00	0.44
1:B:568:LYS:O	1:B:607:GLY:HA3	2.17	0.44
1:A:621:LYS:HA	1:A:621:LYS:HD2	1.86	0.44
1:A:817:ILE:HA	1:A:817:ILE:HD13	1.79	0.44
1:C:817:ILE:HA	1:C:817:ILE:HD13	1.74	0.44
1:A:379:VAL:O	1:A:467:ILE:HD11	2.18	0.44
1:A:53:PHE:CD1	1:A:188:PRO:HG3	2.53	0.44
1:C:567:VAL:HA	1:C:606:GLY:O	2.18	0.44
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.83	0.44
1:B:92:GLY:O	1:B:128:ASP:HA	2.18	0.44
1:B:93:ARG:HH11	1:B:93:ARG:HD3	1.68	0.43
1:D:199:PRO:HB2	1:D:220:VAL:HG13	1.99	0.43
1:D:201:HIS:CD2	1:D:220:VAL:HG22	2.53	0.43
1:A:205:ARG:HD3	1:A:217:ASP:OD2	2.17	0.43
1:D:414:VAL:HG12	1:D:474:LEU:HD22	1.99	0.43
1:C:410:PHE:O	1:C:414:VAL:HG12	2.19	0.43
1:A:513:SER:HB2	1:A:831:ARG:HD3	2.00	0.43
1:C:597:PHE:CE2	1:C:792:LYS:HD3	2.54	0.43
1:C:201:HIS:ND1	1:C:220:VAL:HG22	2.33	0.43
1:B:707:ASN:HA	1:B:800:MET:CE	2.47	0.43
1:C:11:LYS:HE3	1:C:11:LYS:HB2	1.87	0.43
1:B:310:ARG:HH11	2:B:843:AMP:P	2.41	0.43
1:A:363:LYS:HE3	1:A:367:VAL:HG23	2.00	0.43
1:D:628:ASP:O	1:D:632:HIS:HD2	2.01	0.43
1:C:387:TRP:HA	1:C:388:PRO:HD2	1.77	0.43
1:D:778:GLU:O	1:D:782:LYS:HG3	2.19	0.43
1:B:753:LYS:H	1:B:753:LYS:HZ3	1.65	0.43
1:A:754:GLN:HA	1:A:755:PRO:HD2	1.85	0.43
1:B:329:PHE:CE1	1:B:333:VAL:HG21	2.54	0.43
1:B:687:LEU:HD13	1:B:709:PHE:HE2	1.82	0.43
1:B:547:ALA:HB1	1:B:551:ARG:HH22	1.83	0.43
1:A:547:ALA:O	1:A:551:ARG:HG2	2.18	0.43
1:A:304:LEU:O	1:A:308:ILE:HG12	2.19	0.43
1:B:198:LEU:HD22	1:B:305:GLN:OE1	2.18	0.43
1:C:756:ASP:HB3	1:C:759:LYS:HZ3	1.83	0.43
1:B:33:ARG:NH1	1:B:33:ARG:HG2	2.31	0.43
1:D:374:TYR:O	1:D:452:VAL:HA	2.18	0.43
1:A:724:ARG:HH12	1:A:726:TYR:HA	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:ASN:ND2	1:B:72:GLN:HE21	2.17	0.43
1:A:15:VAL:HA	1:A:18:LEU:HD12	2.00	0.43
1:A:577:LEU:HD11	1:A:761:ILE:HD13	2.01	0.42
1:C:159:ILE:CD1	1:C:295:GLN:HG2	2.48	0.42
1:D:233:TYR:HB2	1:D:489:ARG:HD3	2.01	0.42
1:A:34:HIS:O	1:A:38:THR:HB	2.20	0.42
1:C:569:ARG:HG3	1:C:574:LYS:HE3	2.00	0.42
1:C:619:ILE:O	1:C:623:ILE:HG13	2.19	0.42
1:C:169:LYS:O	1:C:176:MET:N	2.51	0.42
1:B:198:LEU:HD13	1:B:305:GLN:HB2	2.01	0.42
1:D:550:GLU:O	1:D:554:LYS:HA	2.19	0.42
1:A:458:ILE:HG22	1:A:462:ILE:CD1	2.49	0.42
1:D:85:LEU:CD1	1:D:303:THR:HG21	2.50	0.42
1:B:413:ARG:HH22	1:B:475:GLU:CD	2.23	0.42
1:C:194:PRO:HG3	1:C:224:MET:HE3	2.01	0.42
1:B:642:VAL:O	1:B:643:ILE:HG13	2.19	0.42
1:A:369:VAL:HA	1:A:448:GLY:O	2.20	0.42
1:A:87:LEU:HD23	1:A:292:ARG:NH2	2.34	0.42
1:B:727:ASN:ND2	1:C:724:ARG:HH21	2.18	0.42
1:D:167:ASN:HD22	1:D:180:ASP:HA	1.84	0.42
1:A:311:PHE:CE1	1:A:323:ARG:HD2	2.54	0.42
1:A:458:ILE:O	1:A:462:ILE:HG13	2.20	0.42
1:B:549:LEU:HD12	1:B:557:ILE:HD13	2.02	0.42
1:B:616:ALA:HA	1:B:619:ILE:HD12	2.00	0.42
1:B:247:LYS:HE3	1:B:247:LYS:HB2	1.74	0.42
1:D:289:LYS:HG3	1:D:291:LEU:H	1.85	0.42
1:A:191:LYS:HG2	1:A:193:ARG:NH2	2.34	0.42
1:C:411:LEU:HA	1:C:414:VAL:CG1	2.50	0.42
1:B:539:GLN:HE21	1:B:543:LEU:HD13	1.84	0.42
1:A:248:ALA:CB	1:A:269:ARG:HA	2.50	0.42
1:D:439:ILE:HA	1:D:439:ILE:HD13	1.87	0.42
1:A:490:ARG:HA	1:A:494:LEU:HB3	2.02	0.42
1:D:69:ARG:HH21	1:D:836:ALA:HB3	1.85	0.42
1:D:94:THR:HB	1:D:189:TRP:CE2	2.55	0.41
1:A:519:ARG:NH1	1:A:807:THR:HG22	2.35	0.41
1:A:381:PRO:HA	1:A:384:LEU:HG	2.00	0.41
1:B:582:HIS:HD2	1:B:781:VAL:HG22	1.84	0.41
1:C:159:ILE:HG22	1:C:160:ARG:N	2.36	0.41
1:A:138:ARG:HH21	1:A:650:VAL:HG11	1.86	0.41
1:D:42:ASP:HB3	1:D:44:ASN:N	2.34	0.41
1:B:571:HIS:H	1:B:576:GLN:HE22	1.68	0.41
1:D:206:VAL:CG2	1:D:398:ARG:HG2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:92:GLY:O	1:C:128:ASP:HA	2.20	0.41
1:C:373:ALA:HA	1:C:449:SER:HB3	2.02	0.41
1:B:740:GLN:O	1:B:744:GLN:HG3	2.20	0.41
1:C:582:HIS:O	1:C:586:LEU:HD22	2.19	0.41
1:D:53:PHE:CE1	1:D:188:PRO:HD3	2.51	0.41
1:C:490:ARG:HA	1:C:494:LEU:HB3	2.02	0.41
1:B:673:ALA:O	1:B:694:GLY:HA2	2.21	0.41
1:D:571:HIS:CD2	1:D:572:GLU:N	2.89	0.41
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.59	0.41
1:D:142:CYS:SG	1:D:487:THR:HG22	2.61	0.41
1:D:475:GLU:HA	1:D:476:PRO:HD2	1.91	0.41
1:D:496:ASN:ND2	1:D:499:LEU:HB2	2.36	0.41
1:C:521:LEU:HB2	1:C:806:ALA:HB2	2.02	0.41
1:B:536:LYS:HB3	1:B:536:LYS:HE2	1.83	0.41
1:B:88:GLU:HB2	1:B:132:GLY:HA2	2.01	0.41
1:A:521:LEU:HB2	1:A:806:ALA:HB2	2.01	0.41
1:C:136:LEU:HD21	1:C:338:ASN:HD22	1.86	0.41
1:D:631:ASN:OD1	1:D:641:ARG:HA	2.21	0.41
1:D:102:LEU:HD23	1:D:104:LEU:CD1	2.51	0.41
1:A:692:MET:HE1	1:A:710:ILE:HG13	2.03	0.41
1:D:571:HIS:CD2	1:D:573:TYR:HD1	2.38	0.41
1:C:87:LEU:HD22	1:C:292:ARG:NH2	2.36	0.41
3:B:860[B]:PDP:H5A2	3:B:860[B]:PDP:O2B	2.21	0.41
1:A:557:ILE:HD13	1:A:557:ILE:HG21	1.90	0.41
1:D:348:GLU:O	1:D:352:VAL:HG23	2.21	0.41
1:D:267:LEU:HD22	1:D:267:LEU:HA	1.87	0.41
1:B:139:LEU:CD2	1:B:377:HIS:HE1	2.34	0.41
1:A:453:ASN:HA	1:A:480:GLN:O	2.21	0.41
1:C:346:ILE:HB	1:C:347:PRO:HD3	2.03	0.41
1:B:560:ASN:HA	1:B:560:ASN:HD22	1.76	0.41
1:C:60:ARG:HD2	1:C:188:PRO:O	2.21	0.41
1:A:205:ARG:HH11	1:A:205:ARG:HD3	1.75	0.40
1:B:265:ALA:HA	1:B:268:ASP:HB2	2.03	0.40
1:D:497:PRO:O	1:D:501:GLU:HB2	2.20	0.40
1:A:562:LEU:HD12	1:A:661:ASP:HB2	2.03	0.40
1:D:465:LYS:HA	1:D:465:LYS:HD3	1.91	0.40
1:C:33:ARG:HH11	1:C:33:ARG:HG2	1.86	0.40
1:A:522:LEU:O	1:A:525:VAL:HG22	2.21	0.40
1:C:291:LEU:O	1:C:295:GLN:HB2	2.21	0.40
1:D:67:TRP:O	1:D:71:GLN:HG2	2.22	0.40
1:A:40:VAL:HG13	1:B:64:VAL:HG13	2.04	0.40
1:B:323:ARG:HH11	1:B:323:ARG:HD3	1.75	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:726:TYR:CE1	1:C:775:ALA:HB2	2.54	0.40
1:C:332:LYS:HD3	1:C:332:LYS:HA	1.99	0.40
1:A:799:ARG:O	1:A:803:ARG:HG3	2.21	0.40
1:B:55:LEU:HD23	1:B:95:LEU:HD21	2.02	0.40
1:B:165:ILE:O	1:B:165:ILE:HG23	2.21	0.40
1:D:798:THR:O	1:D:802:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	795/842 (94%)	733 (92%)	51 (6%)	11 (1%)	16	50
1	B	785/842 (93%)	725 (92%)	52 (7%)	8 (1%)	22	61
1	C	795/842 (94%)	727 (91%)	61 (8%)	7 (1%)	25	64
1	D	795/842 (94%)	746 (94%)	42 (5%)	7 (1%)	25	64
All	All	3170/3368 (94%)	2931 (92%)	206 (6%)	33 (1%)	22	61

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	166	PHE
1	A	322	VAL
1	B	166	PHE
1	B	321	PRO
1	B	322	VAL
1	B	421	ASP
1	B	835	PRO
1	C	16	ARG
1	C	166	PHE
1	C	835	PRO
1	D	16	ARG

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Mol	Chain	Res	Type
1	D	166	PHE
1	D	835	PRO
1	A	552	GLU
1	B	675	GLY
1	D	17	GLY
1	D	199	PRO
1	D	435	ALA
1	D	675	GLY
1	A	16	ARG
1	A	361	TRP
1	B	435	ALA
1	C	551	ARG
1	C	705	GLU
1	A	133	ASN
1	A	321	PRO
1	A	475	GLU
1	A	675	GLY
1	B	484	ASN
1	A	165	ILE
1	C	629	VAL
1	C	379	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	693/731 (95%)	631 (91%)	62 (9%)	14	38
1	B	685/731 (94%)	614 (90%)	71 (10%)	10	27
1	C	693/731 (95%)	614 (89%)	79 (11%)	8	22
1	D	693/731 (95%)	622 (90%)	71 (10%)	11	29
All	All	2764/2924 (94%)	2481 (90%)	283 (10%)	11	29

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG

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Mol	Chain	Res	Type
1	A	15	VAL
1	A	21	VAL
1	A	26	GLU
1	A	27	LEU
1	A	41	LYS
1	A	90	TYR
1	A	122	LEU
1	A	138	ARG
1	A	150	LEU
1	A	162	GLU
1	A	169	LYS
1	A	176	MET
1	A	191	LYS
1	A	193	ARG
1	A	211	GLN
1	A	242	ARG
1	A	264	GLN
1	A	269	ARG
1	A	270	ASN
1	A	273	GLU
1	A	274	ASN
1	A	292	ARG
1	A	315	LYS
1	A	321	PRO
1	A	323	ARG
1	A	359	LEU
1	A	376	ASN
1	A	398	ARG
1	A	411	LEU
1	A	414	VAL
1	A	422	VAL
1	A	433	GLU
1	A	452	VAL
1	A	470	ASP
1	A	473	GLU
1	A	489	ARG
1	A	493	VAL
1	A	499	LEU
1	A	506	ARG
1	A	525	VAL
1	A	542	LYS
1	A	543	LEU

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Mol	Chain	Res	Type
1	A	570	ILE
1	A	578	LEU
1	A	579	ASN
1	A	581	LEU
1	A	583	VAL
1	A	635	VAL
1	A	641	ARG
1	A	649	ARG
1	A	678	ASN
1	A	683	LEU
1	A	702	GLU
1	A	718	VAL
1	A	724	ARG
1	A	751	SER
1	A	753	LYS
1	A	756	ASP
1	A	761	ILE
1	A	764	MET
1	A	832	GLN
1	B	23	ASN
1	B	41	LYS
1	B	48	PRO
1	B	77	LYS
1	B	79	PRO
1	B	87	LEU
1	B	90	TYR
1	B	112	THR
1	B	122	LEU
1	B	138	ARG
1	B	169	LYS
1	B	176	MET
1	B	191	LYS
1	B	193	ARG
1	B	205	ARG
1	B	209	THR
1	B	210	SER
1	B	230	VAL
1	B	242	ARG
1	B	270	ASN
1	B	273	GLU
1	B	291	LEU
1	B	304	LEU

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Mol	Chain	Res	Type
1	B	315	LYS
1	B	321	PRO
1	B	324	THR
1	B	363	LYS
1	B	381	PRO
1	B	398	ARG
1	B	411	LEU
1	B	412	ASN
1	B	433	GLU
1	B	452	VAL
1	B	465	LYS
1	B	473	GLU
1	B	489	ARG
1	B	493	VAL
1	B	496	ASN
1	B	499	LEU
1	B	501	GLU
1	B	505	GLU
1	B	506	ARG
1	B	544	LYS
1	B	550	GLU
1	B	556	HIS
1	B	559	PRO
1	B	562	LEU
1	B	566	GLN
1	B	577	LEU
1	B	578	LEU
1	B	579	ASN
1	B	591	LYS
1	B	592	LYS
1	B	598	VAL
1	B	639	ARG
1	B	649	ARG
1	B	651	SER
1	B	658	PRO
1	B	683	LEU
1	B	706	GLU
1	B	708	PHE
1	B	720	ARG
1	B	724	ARG
1	B	730	GLU
1	B	753	LYS

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Mol	Chain	Res	Type
1	B	761	ILE
1	B	779	GLU
1	B	788	SER
1	B	793	ASN
1	B	834	LEU
1	B	835	PRO
1	C	10	ARG
1	C	15	VAL
1	C	22	GLU
1	C	27	LEU
1	C	41	LYS
1	C	43	ARG
1	C	48	PRO
1	C	77	LYS
1	C	87	LEU
1	C	90	TYR
1	C	113	TYR
1	C	122	LEU
1	C	138	ARG
1	C	144	LEU
1	C	163	PHE
1	C	167	ASN
1	C	169	LYS
1	C	176	MET
1	C	191	LYS
1	C	193	ARG
1	C	205	ARG
1	C	214	LYS
1	C	217	ASP
1	C	242	ARG
1	C	267	LEU
1	C	270	ASN
1	C	274	ASN
1	C	289	LYS
1	C	319	ARG
1	C	339	ASP
1	C	371	THR
1	C	379	VAL
1	C	382	GLU
1	C	389	VAL
1	C	398	ARG
1	C	407	ASN

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Mol	Chain	Res	Type
1	C	412	ASN
1	C	414	VAL
1	C	421	ASP
1	C	438	ARG
1	C	462	ILE
1	C	473	GLU
1	C	489	ARG
1	C	496	ASN
1	C	499	LEU
1	C	510	GLU
1	C	532	ARG
1	C	553	TYR
1	C	555	VAL
1	C	561	SER
1	C	562	LEU
1	C	569	ARG
1	C	577	LEU
1	C	578	LEU
1	C	579	ASN
1	C	586	LEU
1	C	589	ARG
1	C	635	VAL
1	C	643	ILE
1	C	646	GLU
1	C	649	ARG
1	C	683	LEU
1	C	705	GLU
1	C	706	GLU
1	C	708	PHE
1	C	714	ARG
1	C	718	VAL
1	C	724	ARG
1	C	734	ARG
1	C	736	PRO
1	C	753	LYS
1	C	761	ILE
1	C	766	MET
1	C	779	GLU
1	C	827	VAL
1	C	831	ARG
1	C	832	GLN
1	C	833	ARG

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Mol	Chain	Res	Type
1	C	835	PRO
1	D	10	ARG
1	D	15	VAL
1	D	16	ARG
1	D	21	VAL
1	D	23	ASN
1	D	26	GLU
1	D	41	LYS
1	D	42	ASP
1	D	69	ARG
1	D	77	LYS
1	D	87	LEU
1	D	90	TYR
1	D	106	ASN
1	D	122	LEU
1	D	138	ARG
1	D	169	LYS
1	D	191	LYS
1	D	193	ARG
1	D	199	PRO
1	D	205	ARG
1	D	207	GLU
1	D	230	VAL
1	D	242	ARG
1	D	267	LEU
1	D	269	ARG
1	D	273	GLU
1	D	292	ARG
1	D	320	ASP
1	D	323	ARG
1	D	327	ASP
1	D	358	ARG
1	D	360	ASP
1	D	380	LEU
1	D	389	VAL
1	D	390	HIS
1	D	398	ARG
1	D	405	GLU
1	D	408	GLN
1	D	411	LEU
1	D	433	GLU
1	D	452	VAL

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Mol	Chain	Res	Type
1	D	489	ARG
1	D	490	ARG
1	D	496	ASN
1	D	499	LEU
1	D	525	VAL
1	D	543	LEU
1	D	554	LYS
1	D	562	LEU
1	D	576	GLN
1	D	577	LEU
1	D	579	ASN
1	D	581	LEU
1	D	592	LYS
1	D	613	TYR
1	D	618	MET
1	D	635	VAL
1	D	683	LEU
1	D	701	GLU
1	D	702	GLU
1	D	706	GLU
1	D	708	PHE
1	D	724	ARG
1	D	734	ARG
1	D	743	GLU
1	D	753	LYS
1	D	754	GLN
1	D	759	LYS
1	D	761	ILE
1	D	793	ASN
1	D	835	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	36	HIS
1	A	44	ASN
1	A	167	ASN
1	A	201	HIS
1	A	264	GLN
1	A	274	ASN
1	A	295	GLN

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	407	ASN
1	A	484	ASN
1	A	566	GLN
1	A	571	HIS
1	A	579	ASN
1	A	582	HIS
1	A	588	ASN
1	A	684	ASN
1	A	744	GLN
1	A	754	GLN
1	A	832	GLN
1	B	36	HIS
1	B	201	HIS
1	B	407	ASN
1	B	453	ASN
1	B	496	ASN
1	B	517	GLN
1	B	539	GLN
1	B	541	ASN
1	B	556	HIS
1	B	560	ASN
1	B	566	GLN
1	B	571	HIS
1	B	576	GLN
1	B	588	ASN
1	B	614	HIS
1	B	632	HIS
1	B	684	ASN
1	B	740	GLN
1	B	744	GLN
1	B	793	ASN
1	C	12	GLN
1	C	57	HIS
1	C	167	ASN
1	C	208	HIS
1	C	341	HIS
1	C	453	ASN
1	C	477	HIS
1	C	496	ASN
1	C	517	GLN
1	C	539	GLN

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Mol	Chain	Res	Type
1	C	541	ASN
1	C	566	GLN
1	C	571	HIS
1	C	576	GLN
1	C	579	ASN
1	C	582	HIS
1	C	588	ASN
1	C	632	HIS
1	C	684	ASN
1	C	744	GLN
1	C	754	GLN
1	D	12	GLN
1	D	57	HIS
1	D	201	HIS
1	D	264	GLN
1	D	274	ASN
1	D	407	ASN
1	D	412	ASN
1	D	496	ASN
1	D	517	GLN
1	D	539	GLN
1	D	541	ASN
1	D	566	GLN
1	D	571	HIS
1	D	576	GLN
1	D	579	ASN
1	D	632	HIS
1	D	684	ASN
1	D	754	GLN
1	D	804	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	AMP	A	843	-	25,25,25	0.91	1 (4%)	38,38,38	1.00	1 (2%)
3	PDP	A	860[A]	1	18,19,20	2.71	6 (33%)	27,29,30	1.77	8 (29%)
3	PDP	A	860[B]	1	18,19,20	3.06	6 (33%)	27,29,30	1.73	7 (25%)
2	AMP	B	843	-	25,25,25	1.14	1 (4%)	38,38,38	1.29	3 (7%)
3	PDP	B	860[A]	1	18,19,20	2.77	6 (33%)	27,29,30	1.67	6 (22%)
3	PDP	B	860[B]	1	18,19,20	2.80	6 (33%)	27,29,30	2.40	8 (29%)
2	AMP	C	843	-	25,25,25	1.11	1 (4%)	38,38,38	1.31	2 (5%)
3	PDP	C	860[A]	1	18,19,20	3.15	5 (27%)	27,29,30	1.68	5 (18%)
3	PDP	C	860[B]	1	18,19,20	2.85	6 (33%)	27,29,30	1.58	6 (22%)
2	AMP	D	843	-	25,25,25	1.02	2 (8%)	38,38,38	1.56	6 (15%)
3	PDP	D	860[A]	1	18,19,20	2.76	6 (33%)	27,29,30	1.77	7 (25%)
3	PDP	D	860[B]	1	18,19,20	2.89	6 (33%)	27,29,30	1.88	9 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	843	-	-	0/10/26/26	0/1/3/3
3	PDP	A	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	A	860[B]	1	-	0/12/12/14	0/1/1/1
2	AMP	B	843	-	-	0/10/26/26	0/1/3/3
3	PDP	B	860[A]	1	-	0/12/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PDP	B	860[B]	1	-	0/12/12/14	0/1/1/1
2	AMP	C	843	-	-	0/10/26/26	0/1/3/3
3	PDP	C	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	C	860[B]	1	-	0/12/12/14	0/1/1/1
2	AMP	D	843	-	-	0/10/26/26	0/1/3/3
3	PDP	D	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	D	860[B]	1	-	0/12/12/14	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	860[A]	PDP	C3-C2	-7.59	1.35	1.40
3	A	860[B]	PDP	C3-C2	-7.45	1.35	1.40
3	B	860[B]	PDP	PA-O3A	-7.34	1.46	1.59
3	D	860[B]	PDP	PB-O3A	-7.11	1.47	1.60
3	A	860[A]	PDP	PB-O3A	-6.66	1.48	1.60
3	C	860[A]	PDP	PA-O3A	-6.60	1.47	1.59
3	B	860[A]	PDP	PB-O3A	-6.52	1.48	1.60
3	C	860[B]	PDP	PB-O3A	-6.39	1.49	1.60
3	D	860[A]	PDP	PB-O3A	-6.33	1.49	1.60
3	A	860[B]	PDP	PB-O3A	-6.33	1.49	1.60
3	C	860[A]	PDP	PB-O3A	-6.26	1.49	1.60
3	C	860[B]	PDP	C3-C2	-6.23	1.36	1.40
3	D	860[B]	PDP	PA-O3A	-6.21	1.48	1.59
3	A	860[B]	PDP	PA-O3A	-6.18	1.48	1.59
3	B	860[A]	PDP	PA-O3A	-6.16	1.48	1.59
3	B	860[B]	PDP	PB-O3A	-6.13	1.49	1.60
3	D	860[A]	PDP	PA-O3A	-5.98	1.49	1.59
3	C	860[B]	PDP	PA-O3A	-5.97	1.49	1.59
3	A	860[A]	PDP	PA-O3A	-5.58	1.49	1.59
3	D	860[B]	PDP	C3-C2	-5.53	1.36	1.40
3	D	860[A]	PDP	C3-C2	-5.48	1.36	1.40
3	B	860[A]	PDP	C3-C2	-4.94	1.37	1.40
3	A	860[A]	PDP	C3-C2	-4.43	1.37	1.40
3	B	860[B]	PDP	C3-C2	-4.07	1.37	1.40
3	C	860[A]	PDP	PB-O1B	3.73	1.63	1.51
3	B	860[A]	PDP	PB-O1B	3.52	1.63	1.51
3	B	860[B]	PDP	PB-O1B	3.46	1.62	1.51
3	A	860[A]	PDP	PB-O1B	3.38	1.62	1.51
3	A	860[B]	PDP	PB-O1B	3.28	1.62	1.51
3	D	860[A]	PDP	PB-O1B	2.90	1.60	1.51
3	C	860[A]	PDP	PA-O5A	-2.62	1.47	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	860[B]	PDP	PB-O1B	2.58	1.59	1.51
3	B	860[B]	PDP	PA-O1A	2.52	1.61	1.51
3	D	860[A]	PDP	PA-O1A	2.49	1.60	1.51
3	B	860[A]	PDP	PA-O5A	-2.48	1.48	1.59
3	A	860[A]	PDP	PA-O1A	2.44	1.60	1.51
3	C	860[B]	PDP	PA-O5A	-2.42	1.48	1.59
3	D	860[B]	PDP	PB-O1B	2.42	1.59	1.51
3	D	860[A]	PDP	PA-O5A	-2.37	1.48	1.59
3	A	860[B]	PDP	PA-O5A	-2.36	1.48	1.59
3	D	860[B]	PDP	PA-O5A	-2.34	1.48	1.59
2	C	843	AMP	C8-N7	-2.31	1.30	1.34
3	B	860[B]	PDP	PA-O5A	-2.27	1.48	1.59
3	A	860[A]	PDP	PA-O5A	-2.26	1.49	1.59
3	A	860[B]	PDP	PA-O1A	2.20	1.59	1.51
3	C	860[B]	PDP	PA-O1A	2.14	1.59	1.51
3	D	860[B]	PDP	PA-O1A	2.14	1.59	1.51
3	B	860[A]	PDP	PA-O1A	2.12	1.59	1.51
2	B	843	AMP	C2'-C1'	-2.11	1.50	1.53
2	A	843	AMP	C8-N7	-2.09	1.30	1.34
2	D	843	AMP	C8-N7	-2.07	1.30	1.34
2	D	843	AMP	C2'-C1'	-2.01	1.50	1.53

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	860[B]	PDP	O5A-C5A-C5	7.09	123.67	109.26
3	B	860[B]	PDP	PA-O3A-PB	-5.88	114.44	131.68
2	B	843	AMP	O4'-C1'-N9	4.93	113.02	108.44
2	D	843	AMP	O4'-C1'-N9	4.85	112.95	108.44
3	C	860[A]	PDP	PA-O3A-PB	-4.82	117.56	131.68
3	A	860[A]	PDP	PA-O3A-PB	-4.71	117.88	131.68
3	D	860[B]	PDP	PA-O3A-PB	-4.69	117.93	131.68
3	A	860[B]	PDP	PA-O3A-PB	-4.34	118.94	131.68
3	D	860[A]	PDP	PA-O3A-PB	-4.17	119.44	131.68
3	A	860[A]	PDP	O3A-PA-O5A	4.12	121.81	103.41
2	C	843	AMP	O4'-C1'-N9	4.12	112.27	108.44
2	D	843	AMP	P-O5'-C5'	4.06	129.94	118.19
3	B	860[B]	PDP	O3A-PA-O5A	4.04	121.47	103.41
3	B	860[A]	PDP	PA-O3A-PB	-3.95	120.09	131.68
3	A	860[B]	PDP	O3A-PA-O5A	3.91	120.87	103.41
3	D	860[A]	PDP	O3A-PA-O5A	3.84	120.59	103.41
3	B	860[A]	PDP	O3A-PA-O5A	3.81	120.46	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	860[B]	PDP	O3A-PA-O5A	3.72	120.06	103.41
3	C	860[B]	PDP	O3A-PA-O5A	3.60	119.51	103.41
3	C	860[B]	PDP	PA-O3A-PB	-3.57	121.22	131.68
3	C	860[A]	PDP	O3A-PA-O5A	3.55	119.29	103.41
2	C	843	AMP	P-O5'-C5'	3.43	128.11	118.19
3	D	860[B]	PDP	O5A-C5A-C5	3.38	116.14	109.26
2	D	843	AMP	N3-C2-N1	3.25	131.42	128.71
3	B	860[A]	PDP	O3B-PB-O1B	-3.24	99.87	110.44
3	B	860[B]	PDP	O3B-PB-O1B	-3.07	100.42	110.44
3	D	860[B]	PDP	O2B-PB-O1B	-3.03	100.53	110.44
3	A	860[B]	PDP	O2B-PB-O1B	-2.94	100.81	110.44
3	B	860[B]	PDP	O2B-PB-O1B	-2.94	100.83	110.44
3	B	860[B]	PDP	O3B-PB-O3A	2.84	118.63	105.14
3	D	860[A]	PDP	O5A-C5A-C5	2.81	114.98	109.26
3	C	860[B]	PDP	O3B-PB-O1B	-2.75	101.46	110.44
2	B	843	AMP	C8-N9-C4	-2.74	104.81	106.90
3	C	860[B]	PDP	O2B-PB-O3A	2.71	118.01	105.14
3	D	860[B]	PDP	O2A-PA-O1A	-2.69	97.17	112.21
3	B	860[B]	PDP	O2B-PB-O3A	2.69	117.91	105.14
3	D	860[A]	PDP	O2B-PB-O3A	2.62	117.55	105.14
3	A	860[B]	PDP	O3B-PB-O1B	-2.56	102.08	110.44
3	A	860[A]	PDP	O2A-PA-O1A	-2.52	98.16	112.21
2	D	843	AMP	O2P-P-O5'	-2.51	99.72	106.65
3	B	860[B]	PDP	PA-O5A-C5A	2.50	130.23	121.22
3	D	860[B]	PDP	O3B-PB-O3A	2.47	116.83	105.14
2	D	843	AMP	C8-N9-C4	-2.45	105.03	106.90
3	A	860[B]	PDP	C5-C6-N1	-2.42	119.49	123.86
3	C	860[B]	PDP	O2B-PB-O1B	-2.41	102.56	110.44
3	D	860[A]	PDP	O3B-PB-O1B	-2.40	102.58	110.44
3	C	860[A]	PDP	O2B-PB-O3A	2.40	116.53	105.14
3	D	860[B]	PDP	O3B-PB-O1B	-2.40	102.59	110.44
2	B	843	AMP	C3'-C2'-C1'	2.39	104.64	100.91
3	A	860[B]	PDP	O3B-PB-O3A	2.37	116.38	105.14
3	C	860[A]	PDP	O2A-PA-O1A	-2.37	98.98	112.21
2	A	843	AMP	P-O5'-C5'	2.34	124.97	118.19
3	A	860[A]	PDP	O3B-PB-O1B	-2.28	102.98	110.44
3	A	860[A]	PDP	O2B-PB-O1B	-2.27	103.03	110.44
3	B	860[A]	PDP	O2A-PA-O1A	-2.27	99.56	112.21
3	C	860[B]	PDP	C5-C6-N1	-2.25	119.80	123.86
3	C	860[A]	PDP	O3B-PB-O1B	-2.23	103.16	110.44
3	A	860[A]	PDP	O3B-PB-O3A	2.22	115.68	105.14
3	D	860[A]	PDP	O2A-PA-O1A	-2.20	99.91	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	860[A]	PDP	O3B-PB-O3A	2.20	115.58	105.14
3	B	860[A]	PDP	O2B-PB-O3A	2.20	115.57	105.14
3	A	860[A]	PDP	O2B-PB-O3A	2.18	115.47	105.14
3	A	860[A]	PDP	O3B-PB-O2B	2.17	116.07	107.61
3	A	860[B]	PDP	O2A-PA-O1A	-2.08	100.58	112.21
3	D	860[B]	PDP	O2B-PB-O3A	2.08	115.02	105.14
3	B	860[A]	PDP	O2A-PA-O3A	2.07	114.95	105.14
2	D	843	AMP	C5-C6-N6	2.04	125.33	120.72
3	D	860[B]	PDP	O2A-PA-O3A	2.04	114.80	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.